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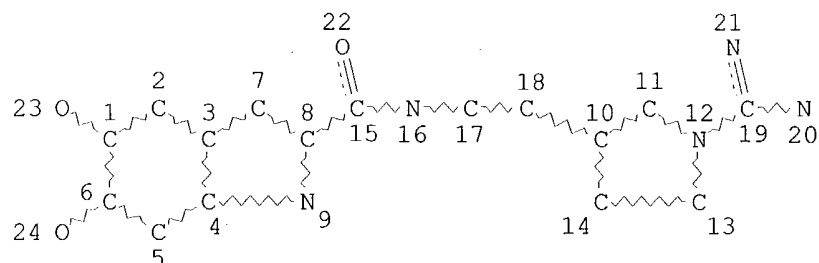
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FILE COVERS 1907 - 10 Nov 2004 VOL 141 ISS 20  
 FILE LAST UPDATED: 9 Nov 2004 (20041109/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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 L3 STR



NODE ATTRIBUTES:  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 24

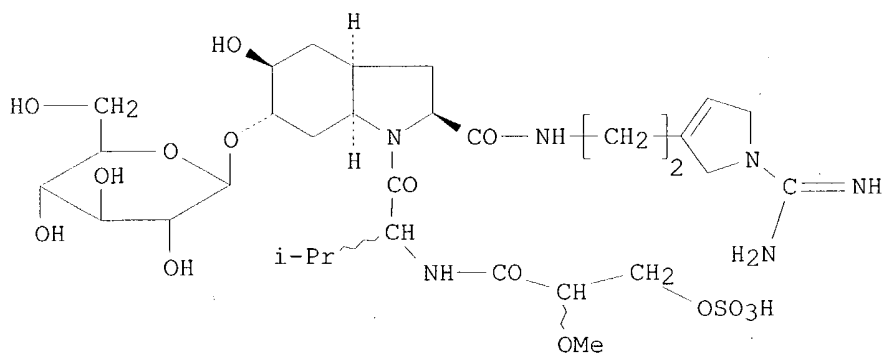
STEREO ATTRIBUTES: NONE  
 L5 8 SEA FILE=REGISTRY SSS FUL L3  
 L6 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L5

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=> d ibib abs hitstr l6 1-5

L6 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2004:553526 HCAPLUS  
 DOCUMENT NUMBER: 141:221980  
 TITLE: Dysinosins B-D, inhibitors of factor VIIa and thrombin from the Australian sponge *Lamellodysidea chlorea*  
 AUTHOR(S): Carroll, Anthony R.; Buchanan, Malcolm S.; Edser, Annette; Hyde, Edward; Simpson, Moana; Quinn, Ronald J.  
 CORPORATE SOURCE: Natural Product Discovery, Eskitis Institute, Griffith University, Brisbane, 4111, Australia  
 SOURCE: Journal of Natural Products (2004), 67(8), 1291-1294  
 CODEN: JNPRDF; ISSN: 0163-3864  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB Three new marine natural products, dysinosins B-D (e.g. I, dysinosin B), were isolated from the sponge *Lamellodysidea chlorea* and their structures determined by 1D and 2D NMR spectroscopy. These compds. are inhibitors of the blood coagulation cascade serine proteases factor VIIa and thrombin. These analogs, dysinosins B-D, allowed identification of two structural motifs within the structures that contribute to binding to the proteases, factor VIIa and thrombin.

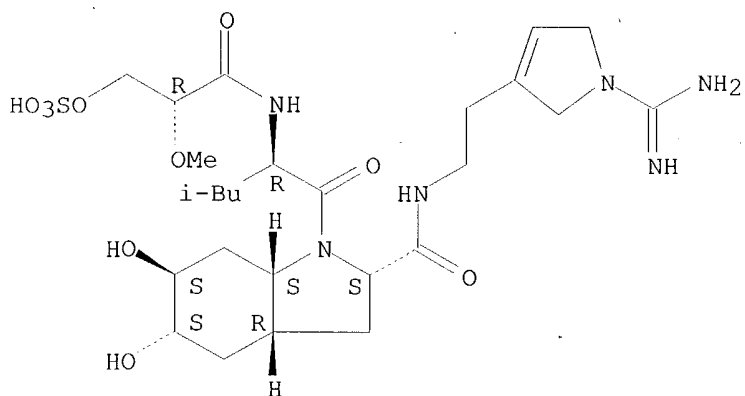
IT 477708-72-8, Dysinosin A

RL: BSU (Biological study, unclassified); BIOL (Biological study)  
 (inhibitors of factor VIIa and thrombin from Australian sponge  
*Lamellodysidea chlorea*)

RN 477708-72-8 HCAPLUS

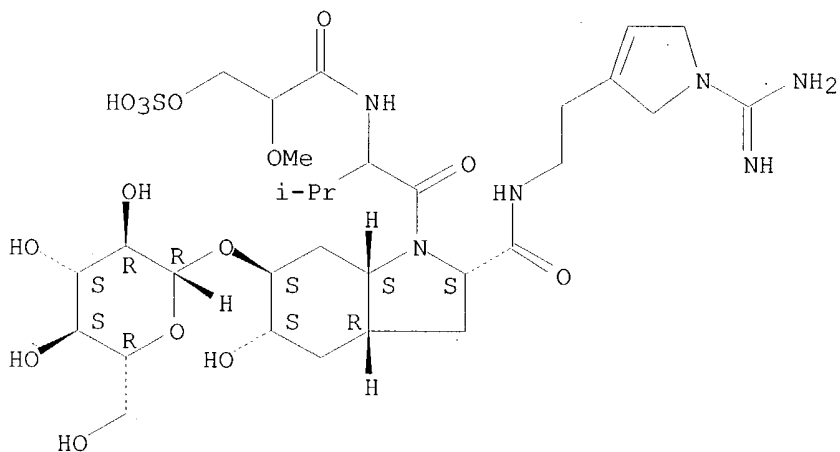
CN 1H-Indole-2-carboxamide, N-[2-[1-(aminoiminomethyl)-2,5-dihydro-1H-pyrrol-3-yl]ethyl]octahydro-5,6-dihydroxy-1-[(2R)-2-[[ (2R)-2-methoxy-1-oxo-3-(sulfooxy)propyl]amino]-4-methyl-1-oxopentyl]-, (2S,3aR,5S,6S,7aS)- (9CI)  
 (CA INDEX NAME)

Absolute stereochemistry.



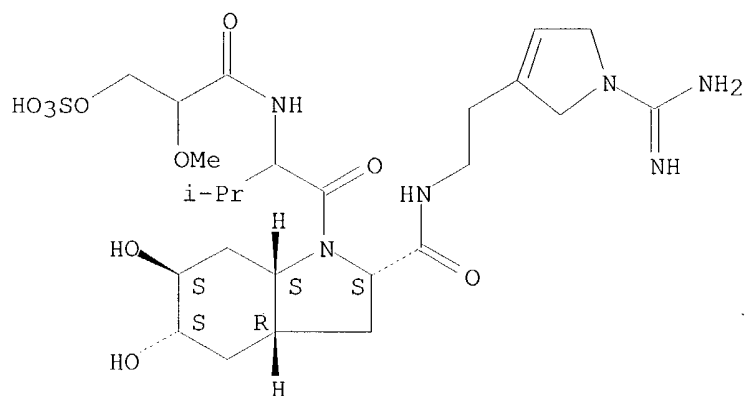
IT 745826-09-9P, Dysynosin B 745826-10-2P, Dysynosin C  
 745826-11-3P, Dysynosin D  
 RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)  
 (inhibitors of factor VIIa and thrombin from Australian sponge *Lamellodysidea chlorea*)  
 RN 745826-09-9 HCAPLUS  
 CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry. Rotation (+).  
 Currently available stereo shown.



RN 745826-10-2 HCAPLUS  
 CN 1H-Indole-2-carboxamide, N-[2-[1-(aminoiminomethyl)-2,5-dihydro-1H-pyrrol-3-yl]ethyl]octahydro-5,6-dihydroxy-1-[2-[[2-methoxy-1-oxo-3-(sulfoxy)propyl]amino]-3-methyl-1-oxobutyl]-, (2S,3aR,5S,6S,7aS)- (9CI)  
 (CA INDEX NAME)

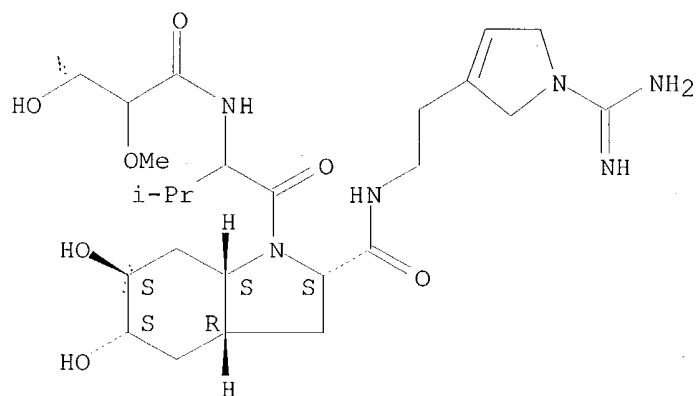
Absolute stereochemistry.  
 Currently available stereo shown.



RN 745826-11-3 HCAPLUS

CN 1H-Indole-2-carboxamide, N-[2-[1-(aminoiminomethyl)-2,5-dihydro-1H-pyrrol-3-yl]ethyl]octahydro-5,6-dihydroxy-1-[2-[(3-hydroxy-2-methoxy-1-oxopropyl)amino]-3-methyl-1-oxobutyl]-, (2S,3aR,5S,6S,7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Currently available stereo shown.



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:491178 HCAPLUS

DOCUMENT NUMBER: 139:47155

TITLE: Protease inhibitors of the coagulation cascade isolated from dysidea sponges

INVENTOR(S): Goetz, Gilles H.; Harrigan, George G.; Likos, John J.; Kasten, Thomas P.

PATENT ASSIGNEE(S): Pharmacia Corporation, USA

SOURCE: PCT Int. Appl., 38 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003051831	A2	20030626	WO 2002-US40001	20021213
WO 2003051831	A3	20031030		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003158248	A1	20030821	US 2002-307803	20021202
US 6716869	B2	20040406		
EP 1465866	A2	20041013	EP 2002-782410	20021213
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
US 2004147456	A1	20040729	US 2004-759667	20040116
PRIORITY APPLN. INFO.:				
			US 2001-341527P	P 20011217
			US 2002-307803	A 20021202
			WO 2002-US40001	W 20021213

AB The present invention is directed toward a composition comprising a compound isolated from Dysidea species sponges that is capable of inhibiting serine proteases of the coagulation cascade. In particular, this composition inhibits the TF/VIIa complex of the coagulation cascade. The invention is also directed toward methods employing this composition as a part of anticoagulant therapy.

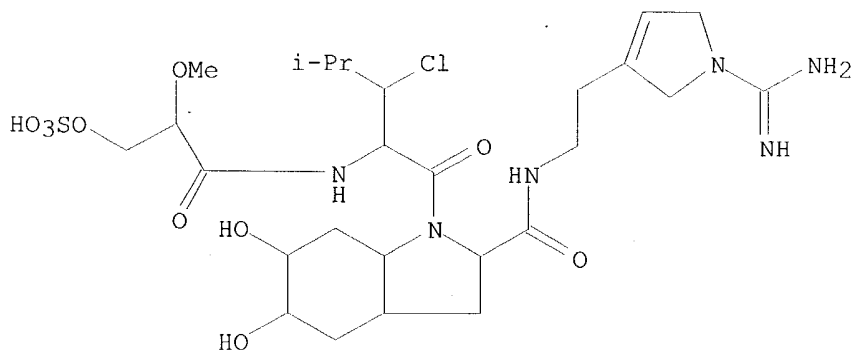
IT **548443-14-7P**

RL: NPO (Natural product occurrence); PAC (Pharmacological activity); PRP (Properties); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); USES (Uses)  
 (protease inhibitors of coagulation cascade isolated from dysidea sponges for anticoagulant therapy in combination with thrombolytic agents)

RN 548443-14-7 HCAPLUS

CN 1H-Indole-2-carboxamide, N-[2-[1-(aminoiminomethyl)-2,5-dihydro-1H-pyrrol-3-yl]ethyl]-1-[3-chloro-2-[[2-methoxy-1-oxo-3-(sulfooxy)propyl]amino]-4-methyl-1-oxopentyl]octahydro-5,6-dihydroxy- (9CI) (CA INDEX NAME)

Currently available stereo shown.



RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(protease inhibitors of coagulation cascade isolated from dysidea sponges for anticoagulant therapy in combination with thrombolytic agents

L6 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:321340 HCAPLUS

DOCUMENT NUMBER: 139:149881

TITLE: New and old challenges in total synthesis. From concept to practice

AUTHOR(S): Hanessian, Stephen; Margarita, Roberto; Hall, Adrian; Johnstone, Shawn; Tremblay, Martin; Parlanti, Luca

CORPORATE SOURCE: Department of Chemistry, Universite de Montreal, Montreal, QC, H3C 3J, Can.

SOURCE: Pure and Applied Chemistry (2003), 75(2-3), 209-221  
CODEN: PACHAS; ISSN: 0033-4545

PUBLISHER: International Union of Pure and Applied Chemistry

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB A review. The total synthesis of dysynosin A, a novel member of the aeruginosin group of marine natural products, is discussed. The stereocontrolled synthesis also confirms the proposed structure and absolute stereochem. of the natural product.

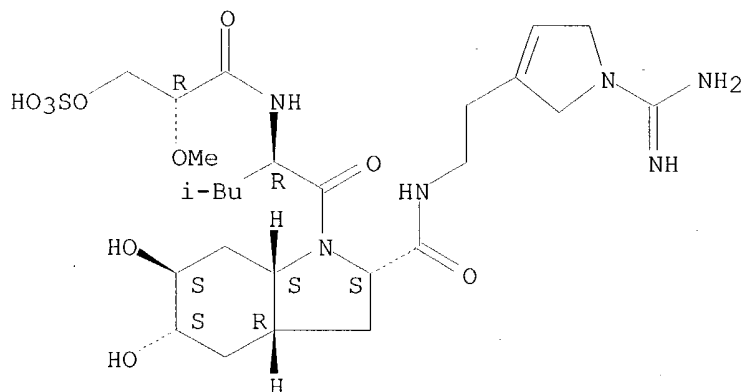
IT 477708-72-8P, Dysynosin A

RL: SPN (Synthetic preparation); PREP (Preparation)  
(total synthesis of dysynosin A and confirmation of its structure and stereochem.)

RN 477708-72-8 HCAPLUS

CN 1H-Indole-2-carboxamide, N-[2-[1-(aminoiminomethyl)-2,5-dihydro-1H-pyrrol-3-yl]ethyl]octahydro-5,6-dihydroxy-1-[(2R)-2-[(2R)-2-methoxy-1-oxo-3-(sulfooxy)propyl]amino]-4-methyl-1-oxopentyl]-, (2S,3aR,5S,6S,7aS)- (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 79 THERE ARE 79 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN

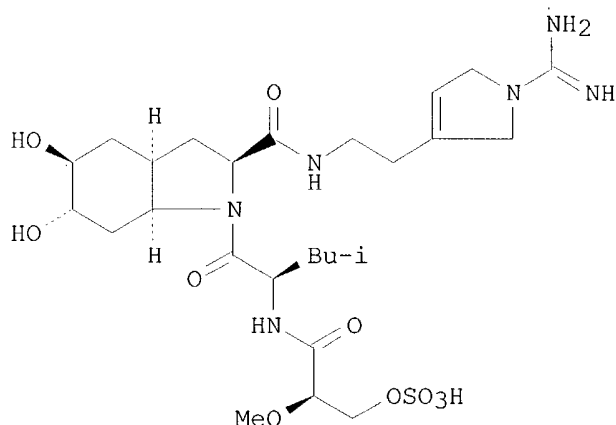
ACCESSION NUMBER: 2002:789748 HCAPLUS

DOCUMENT NUMBER: 138:14174

TITLE: Total synthesis and structural confirmation of the marine natural product dysynosin A: a novel inhibitor of thrombin and factor VIIa

AUTHOR(S): Hanessian, Stephen; Margarita, Roberto; Hall, Adrian;

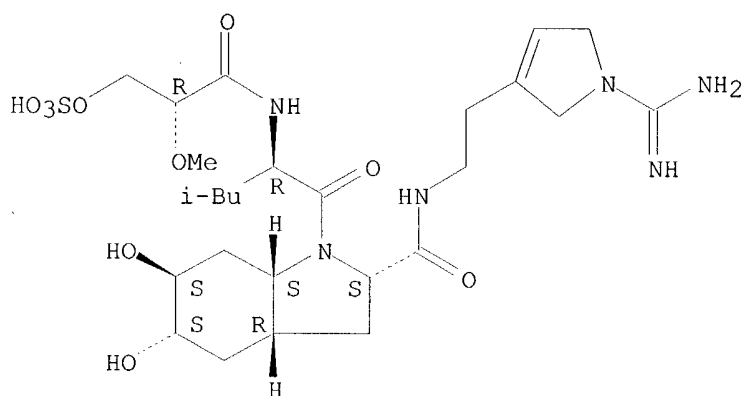
CORPORATE SOURCE: Johnstone, Shawn; Tremblay, Martin; Parlanti, Luca  
 Department of Chemistry, Universite de Montreal,  
 Montreal, QC, H3C 3J7, Can.  
 SOURCE: Journal of the American Chemical Society (2002),  
 124(45), 13342-13343  
 CODEN: JACSAT; ISSN: 0002-7863  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 138:14174  
 GI



I

- AB The structure and absolute configuration of the marine antithrombotic product dysinosin A (I) was confirmed by total synthesis. The strategy involved disconnection to three subunits, of which two were synthesized from the readily available L-glutamic acid, D-leucine, and D-mannitol. The Grubbs olefin metathesis carbo cyclization reaction was utilized to prepare two intermediates.
- IT **477708-72-8P**, Dysinosin A  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (total synthesis from amino acids via Grubbs olefin metathesis carbo cyclization of marine natural product dysinosin A, its crystal structure and absolute configuration)
- RN 477708-72-8 HCAPLUS
- CN 1H-Indole-2-carboxamide, N-[2-[1-(aminoiminomethyl)-2,5-dihydro-1H-pyrrol-3-yl]ethyl]octahydro-5,6-dihydroxy-1-[(2R)-2-[[2-(2-methoxy-1-oxo-3-(sulfoxy)propyl)amino]-4-methyl-1-oxopentyl]-, (2S,3aR,5S,6S,7aS)- (9CI)  
 (CA INDEX NAME)

Absolute stereochemistry.



IT 477351-68-1P 477351-69-2P 477351-81-8P

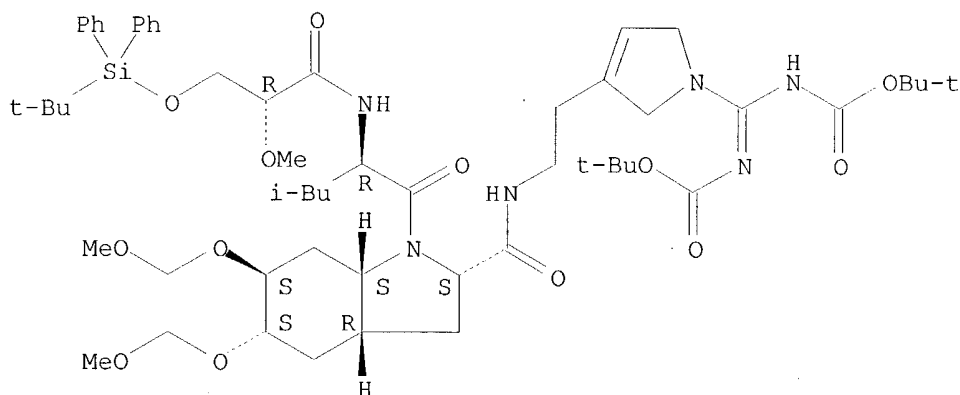
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(total synthesis from amino acids via Grubbs olefin metathesis carbocyclization reaction of marine natural product dysinosin A, its crystal structure and absolute configuration)

RN 477351-68-1 HCAPLUS

CN Carbamic acid, [[[(1,1-dimethylethoxy)carbonyl]amino][3-[2-[[[(2S,3aR,5S,6S,7aS)-1-[(2R)-2-[[[(2R)-3-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]-2-methoxy-1-oxopropyl]amino]-4-methyl-1-oxopentyl]octahydro-5,6-bis(methoxymethoxy)-1H-indol-2-yl]carbonyl]amino]ethyl]-2,5-dihydro-1H-pyrrol-1-yl]methylene]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

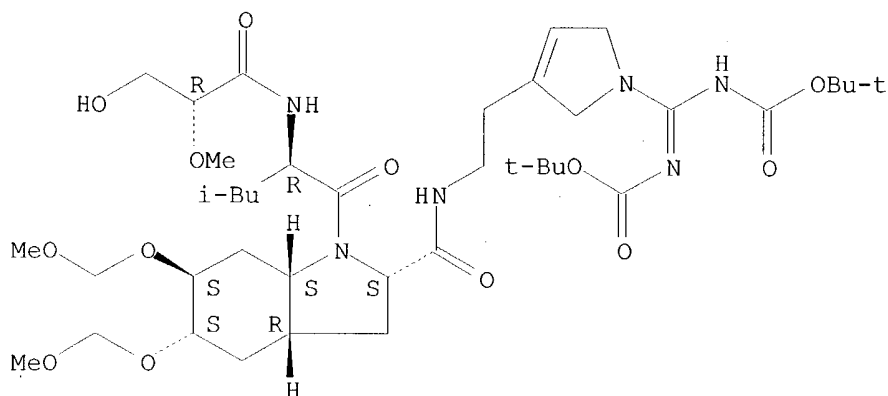


RN 477351-69-2 HCAPLUS

CN Carbamic acid, [[2,5-dihydro-3-[2-[[[(2S,3aR,5S,6S,7aS)-octahydro-1-[(2R)-2-[[[(2R)-3-hydroxy-2-methoxy-1-oxopropyl]amino]-4-methyl-1-oxopentyl]-5,6-bis(methoxymethoxy)-1H-indol-2-yl]carbonyl]amino]ethyl]-1H-pyrrol-1-yl] [[[(1,1-dimethylethoxy)carbonyl]amino]methylene]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

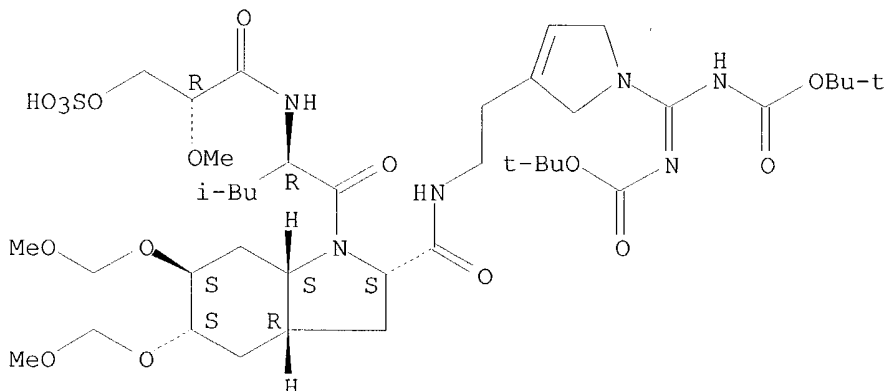




RN 477351-81-8 HCAPLUS

CN Carbamic acid, [[2,5-dihydro-3-[2-[[[(2S,3aR,5S,6S,7aS)-octahydro-5,6-bis(methoxymethoxy)-1-[(2R)-2-[[[(2R)-2-methoxy-1-oxo-3-(sulfooxy)propyl]amino]-4-methyl-1-oxopentyl]-1H-indol-2-yl]carbonyl]amino]ethyl]-1H-pyrrol-1-yl]][(1,1-dimethylethoxy)carbonyl]amino]methylene]-, C-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 72 THERE ARE 72 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:789746 HCAPLUS

DOCUMENT NUMBER: 138:22307

TITLE: Dysinosin A: A novel inhibitor of factor VIIa and thrombin from a new genus and species of Australian sponge of the family Dysideidae

AUTHOR(S): Carroll, Anthony R.; Pierens, Gregory K.; Fechner, Greg; de Leone, Priscila; Ngo, Anna; Simpson, Moana; Hyde, Edward; Hooper, John N. A.; Bostroem, Stig-Lennart; Musil, Djordje; Quinn, Ronald J.

CORPORATE SOURCE: AstraZeneca R&D, Griffith University, Brisbane, 4111, Australia

SOURCE: Journal of the American Chemical Society (2002), 124(45), 13340-13341

PUBLISHER: CODEN: JACSAT; ISSN: 0002-7863  
 DOCUMENT TYPE: American Chemical Society  
 LANGUAGE: Journal  
 English

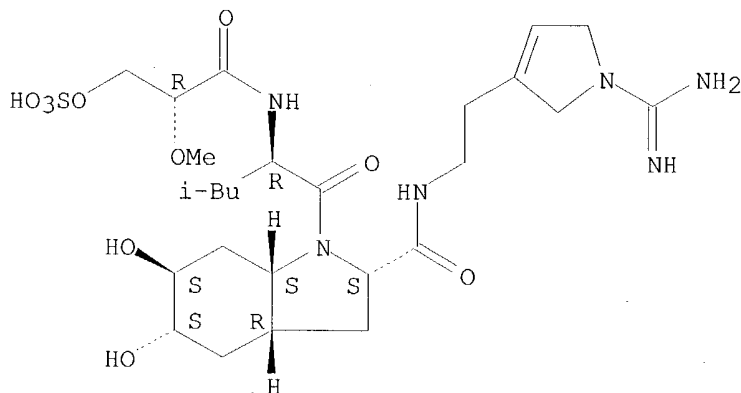
AB A new marine natural product dysinosin A has been isolated from a new genus and species of sponge of the family Dysideidae found near Lizard Island, North Queensland, Australia. Dysinosin A is a potent inhibitor of the blood coagulation cascade factor VIIa and an inhibitor of the serine protease thrombin. Among the distinctive features of dysinosin A are the presence of a 5,6-dihydroxy-octahydroindole-2-carboxylic acid, 3-amino-Et 1-N-amidino-Δ-3-pyrroline, a sulfated glyceric acid, and D-leucine, assembled through three peptidic linkages. Dysinosin A inhibited factor VIIa at a  $K_i$  of 108 nM and thrombin at a  $K_i$  of 452 nM. The identification of the 1-N-amidino-Δ-3-pyrroline and 5,6-dihydroxy-octahydroindole-2-carboxylic acid as P1 and P2 moieties resp., should pave the way for the design and synthesis of new structure-based inhibitors.

IT **477708-72-8P**, Dysinosin A  
 RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)  
 (inhibitor of factor VIIa and thrombin from Australian sponge of family Dysideidae)

RN 477708-72-8 HCAPLUS

CN 1H-Indole-2-carboxamide, N-[2-[1-(aminoiminomethyl)-2,5-dihydro-1H-pyrrol-3-yl]ethyl]octahydro-5,6-dihydroxy-1-[(2R)-2-[[ (2R)-2-methoxy-1-oxo-3-(sulfooxy)propyl]amino]-4-methyl-1-oxopentyl]-, (2S,3aR,5S,6S,7aS)- (9CI)  
 (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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=> fil reg

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STRUCTURE FILE UPDATES: 8 NOV 2004 HIGHEST RN 777024-10-9  
 DICTIONARY FILE UPDATES: 8 NOV 2004 HIGHEST RN 777024-10-9

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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 information enter HELP PROP at an arrow prompt in the file or refer  
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<http://www.cas.org/ONLINE/DBSS/registryss.html>

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L5 ANSWER 1 OF 8 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 745826-11-3 REGISTRY  
 CN 1H-Indole-2-carboxamide, N-[2-[1-(aminoiminomethyl)-2,5-dihydro-1H-pyrrol-  
 3-yl]ethyl]octahydro-5,6-dihydroxy-1-[2-[(3-hydroxy-2-methoxy-1-  
 oxopropyl)amino]-3-methyl-1-oxobutyl]-, (2S,3aR,5S,6S,7aS)- (9CI) (CA  
 INDEX NAME)

OTHER NAMES:

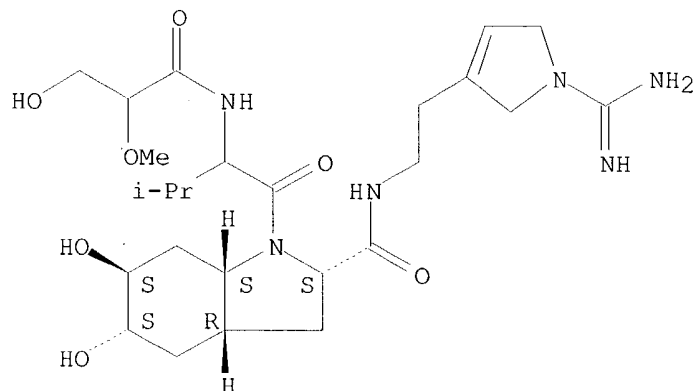
CN Dysinosin D  
 FS STEREOSEARCH  
 MF C25 H42 N6 O7  
 SR CA

LC STN Files: CA, CAPLUS

DT.CA Caplus document type: Journal

RL.NP Roles from non-patents: BIOL (Biological study); OCCU (Occurrence);  
 PREP (Preparation); PRP (Properties)

Absolute stereochemistry.  
 Currently available stereo shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

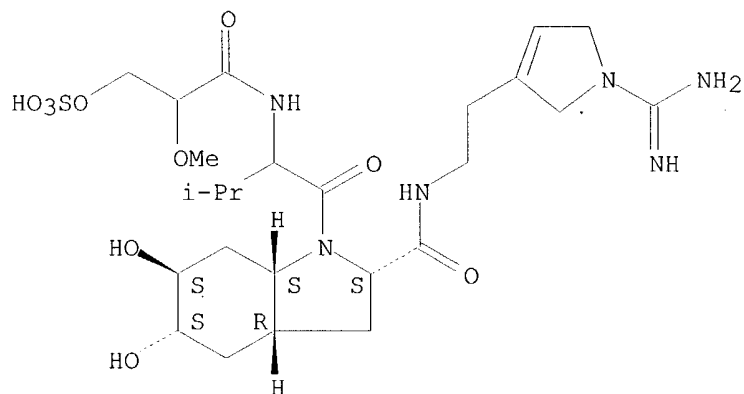
REFERENCE 1: 141:221980

L5 ANSWER 2 OF 8 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 745826-10-2 REGISTRY  
CN 1H-Indole-2-carboxamide, N-[2-[1-(aminoiminomethyl)-2,5-dihydro-1H-pyrrol-3-yl]ethyl]octahydro-5,6-dihydroxy-1-[2-[[2-methoxy-1-oxo-3-(sulfooxy)propyl]amino]-3-methyl-1-oxobutyl]-, (2S,3aR,5S,6S,7aS)- (9CI)  
(CA INDEX NAME)

OTHER NAMES:

CN Dysinosin C  
FS STEREOSEARCH  
MF C25 H42 N6 O10 S  
SR CA  
LC STN Files: CA, CAPLUS  
DT.CA CAplus document type: Journal  
RL.NP Roles from non-patents: BIOL (Biological study); OCCU (Occurrence);  
PREP (Preparation); PRP (Properties)

Absolute stereochemistry.  
Currently available stereo shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:221980

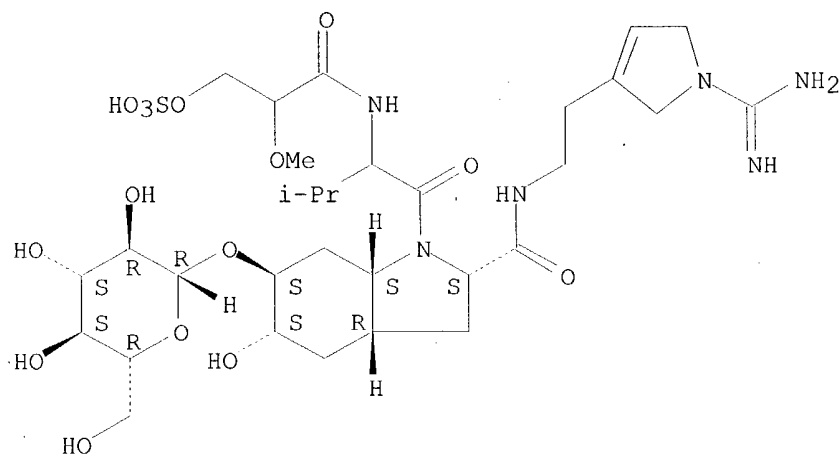
L5 ANSWER 3 OF 8 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 745826-09-9 REGISTRY  
CN INDEX NAME NOT YET ASSIGNED  
OTHER NAMES:  
CN Dysinosin B  
FS STEREOSEARCH  
MF C31 H52 N6 O15 S  
SR CA

LC STN Files: CA, CAPLUS

DT.CA Caplus document type: Journal

RL.NP Roles from non-patents: BIOL (Biological study); OCCU (Occurrence);  
PREP (Preparation); PRP (Properties)

Absolute stereochemistry. Rotation (+).  
Currently available stereo shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:221980

L5 ANSWER 4 OF 8 REGISTRY COPYRIGHT 2004 ACS on STN

RN 548443-14-7 REGISTRY

CN 1H-Indole-2-carboxamide, N-[2-[1-(aminoiminomethyl)-2,5-dihydro-1H-pyrrol-3-yl]ethyl]-1-[3-chloro-2-[[2-methoxy-1-oxo-3-(sulfooxy)propyl]amino]-4-methyl-1-oxopentyl]octahydro-5,6-dihydroxy- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

DR 548443-15-8

MF C26 H43 Cl N6 O10 S

SR CA

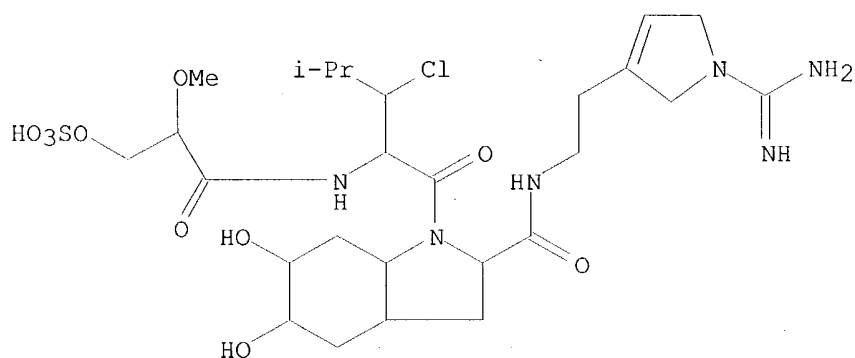
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL

DT.CA Caplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PRP (Properties); USES (Uses)

RLD.P Roles for non-specific derivatives from patents: BIOL (Biological study); USES (Uses)

Currently available stereo shown.



2 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

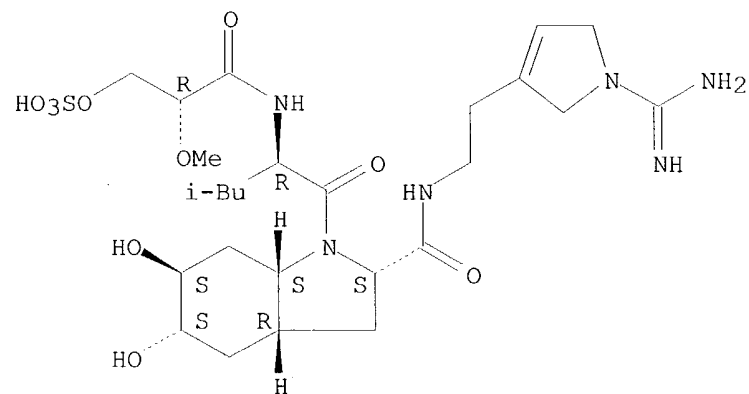
REFERENCE 1: 139:47155

L5 ANSWER 5 OF 8 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 477708-72-8 REGISTRY  
 CN 1H-Indole-2-carboxamide, N-[2-[1-(aminoiminomethyl)-2,5-dihydro-1H-pyrrol-3-yl]ethyl]octahydro-5,6-dihydroxy-1-[(2R)-2-[[ (2R)-2-methoxy-1-oxo-3-(sulfooxy)propyl]amino]-4-methyl-1-oxopentyl]-, (2S,3aR,5S,6S,7aS)- (9CI)  
 (CA INDEX NAME)

OTHER NAMES:

CN Dysinosin A  
 FS STEREOSEARCH  
 MF C26 H44 N6 O10 S  
 SR CA  
 LC STN Files: BIOSIS, CA, CAPLUS, CASREACT, EMBASE, SYNTHLINE  
 DT.CA CAPlus document type: Journal  
 RL.NP Roles from non-patents: BIOL (Biological study); OCCU (Occurrence);  
 PREP (Preparation); PRP (Properties)

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1907 TO DATE)  
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:221980

REFERENCE 2: 139:149881

REFERENCE 3: 138:22307

REFERENCE 4: 138:14174

L5 ANSWER 6 OF 8 REGISTRY COPYRIGHT 2004 ACS on STN

RN 477351-81-8 REGISTRY

CN Carbamic acid, [[2,5-dihydro-3-[2-[[[(2S,3aR,5S,6S,7aS)-octahydro-5,6-bis(methoxymethoxy)-1-[(2R)-2-[[[(2R)-2-methoxy-1-oxo-3-(sulfooxy)propyl]amino]-4-methyl-1-oxopentyl]-1H-indol-2-yl]carbonyl]amino]ethyl]-1H-pyrrol-1-yl]][(1,1-dimethylethoxy)carbonyl]amino]methylene]-, C-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C40 H68 N6 O16 S

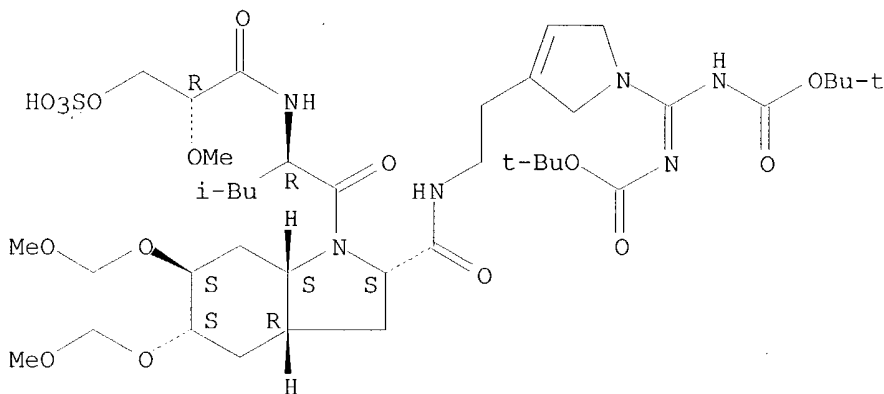
SR CA

LC STN Files: CA, CAPLUS, CASREACT

DT.CA Caplus document type: Journal

RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:14174

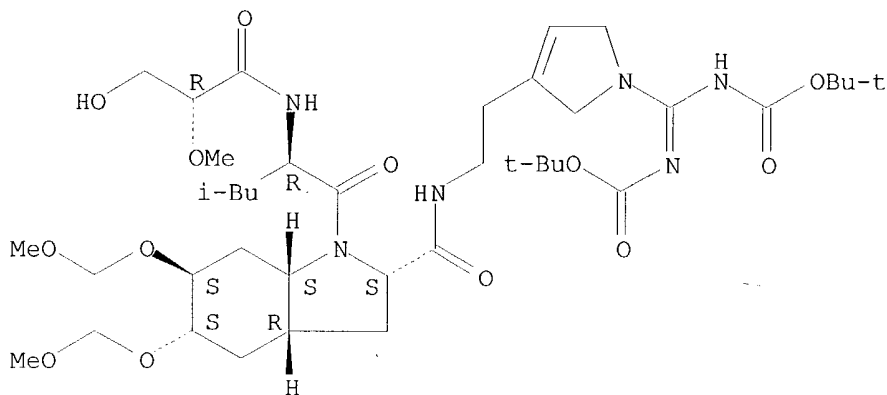
L5 ANSWER 7 OF 8 REGISTRY COPYRIGHT 2004 ACS on STN

RN 477351-69-2 REGISTRY

CN Carbamic acid, [[2,5-dihydro-3-[2-[[[(2S,3aR,5S,6S,7aS)-octahydro-1-[(2R)-2-[[[(2R)-3-hydroxy-2-methoxy-1-oxopropyl]amino]-4-methyl-1-oxopentyl]-5,6-bis(methoxymethoxy)-1H-indol-2-yl]carbonyl]amino]ethyl]-1H-pyrrol-1-

yl][[(1,1-dimethylethoxy)carbonyl]amino]methylene]-, 1,1-dimethylethyl  
 ester (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C40 H68 N6 O13  
 SR CA  
 LC STN Files: CA, CAPLUS, CASREACT  
 DT.CA Caplus document type: Journal  
 RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

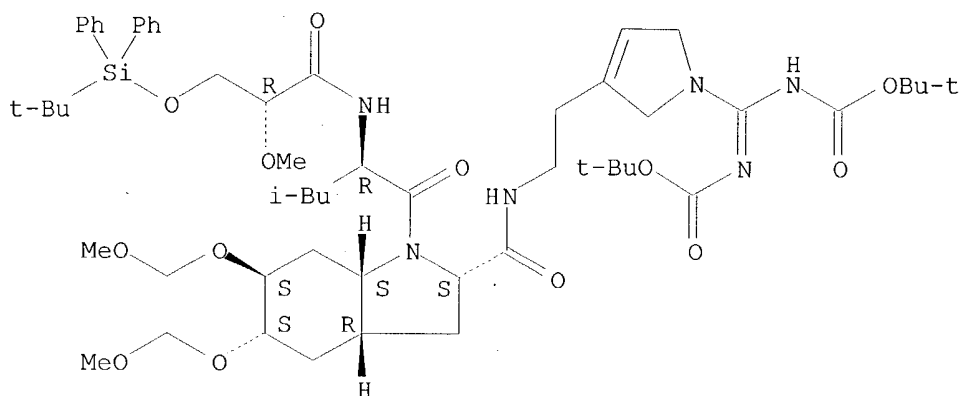
1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:14174

L5 ANSWER 8 OF 8 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 477351-68-1 REGISTRY  
 CN Carbamic acid, [[[(1,1-dimethylethoxy)carbonyl]amino][3-[2-  
 [[[(2S,3aR,5S,6S,7aS)-1-[(2R)-2-[[[(2R)-3-[[[(1,1-  
 dimethylethyl)diphenylsilyl]oxy]-2-methoxy-1-oxopropyl]amino]-4-methyl-1-  
 oxopentyl]octahydro-5,6-bis(methoxymethoxy)-1H-indol-2-  
 yl]carbonyl]amino]ethyl]-2,5-dihydro-1H-pyrrol-1-yl]methylene]-,  
 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C56 H86 N6 O13 Si  
 SR CA  
 LC STN Files: CA, CAPLUS, CASREACT  
 DT.CA Caplus document type: Journal  
 RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

Absolute stereochemistry.





\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:14174

=> □

=> fil beil

FILE 'BEILSTEIN' ENTERED AT 11:30:44 ON 10 NOV 2004

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licensed to Beilstein GmbH and MDL Information Systems GmbH

FILE RELOADED ON OCTOBER 20, 2002

FILE LAST UPDATED ON NOVEMBER 3, 2004

FILE COVERS 1771 TO 2004.

\*\*\* FILE CONTAINS 9,073,068 SUBSTANCES \*\*\*

>>>PLEASE NOTE: Reaction Data and substance data are stored in  
separate documents and can not be searched together in one query.  
Reaction data for BEILSTEIN compounds may be displayed  
immediately with the display codes PRE (preparations) and REA  
(reactions). A substance answer set retrieved after the search  
for a chemical name, a compounds with available reaction  
information by combining with PRE/FA, REA/FA or more generally  
with RX/FA. The BEILSTEIN Registry Number (BRN) is the link  
between a BEILSTEIN compound and belonging reactions. For mo  
detailed reaction searches BRNs can be searched as reaction  
partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

\*\*\*\*\*  
\* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. \*  
\* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE \*  
\* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE \*  
\* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. \*  
\* FOR PRICE INFORMATION SEE HELP COST \*  
\*\*\*\*\*

NEW

- \* PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE SEARCHED, SELECTED AND TRANSFERRED.
- \* NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES, ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A COMPOUND AT A GLANCE.

=>

=> d stat que nos

L3 STR

L5 8 SEA FILE=REGISTRY SSS FUL L3

L7 3 SEA FILE=BEILSTEIN SSS FUL L3

L8 3 SEA FILE=BEILSTEIN ABB=ON PLU=ON L7 NOT L5

=>

=> d brn cn mf fw ctype str rx 1-3

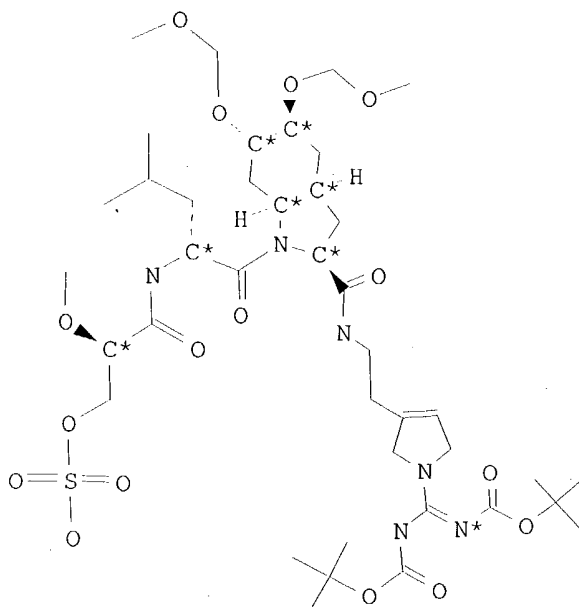
L8 ANSWER 1 OF 3 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN): 9315975  
 Molecular Formula (MF): C40 H68 N6 O16 S . C5 H5 N  
 Molecular Weight (MW): 921.07, 79.10  
 Compound Type (CTYPE): heterocyclic

CM 1

FBRN 9314492

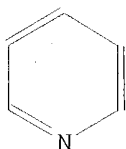
FMF C40 H68 N6 O16 S



CM 2

FBRN 103233

FMF C5 H5 N



## Reaction:

RX

Reaction ID (.ID): 9194848  
 Reactant BRN (.RBRN): 9313827, 3704116  
 Reactant (.RCT): (tert-butoxycarbonylimino-<3-<2-(<1-<2-(3-hydroxy-2-methoxy-propionylamino)-4-methyl-pentanoyl>-5,6-bis-methoxymethoxy-octahydro-indole-2-carbonyl>-amino)-ethyl>-2,5-dihydro-pyrrol-1-yl>-methyl)-carbamic acid tert-butyl ester, pyridine; compound with sulfur trioxide  
 Product BRN (.PBRN): 9315975  
 Product (.PRO): C40H68N6O16S\*C5H5N  
 No. of React. Details (.NVAR): 1

## Reaction Details:

RX

Reaction RID (.RID): 9194848.1  
 Reaction Classification (.CL): Preparation  
 Reagent (.RGT): dibutyltin oxide  
 Solvent (.SOL): CH2Cl2  
 Time (.TIM): 6 hour(s)  
 Reference(s):  
 1. Hanessian, Stephen; Margarita, Roberto; Hall, Adrian; Johnstone, Shawn; Tremblay, Martin; Parlanti, Luca, J.Amer.Chem.Soc., CODEN: JACSAT, 124(45), <2002>, 13342 - 13343; BABS-6373650

## Reaction:

RX

Reaction ID (.ID): 9232324  
 Reactant BRN (.RBRN): 9315975  
 Reactant (.RCT): C40H68N6O16S\*C5H5N  
 Product BRN (.PBRN): 9311246  
 Product (.PRO): dysinosin A  
 No. of React. Details (.NVAR): 1

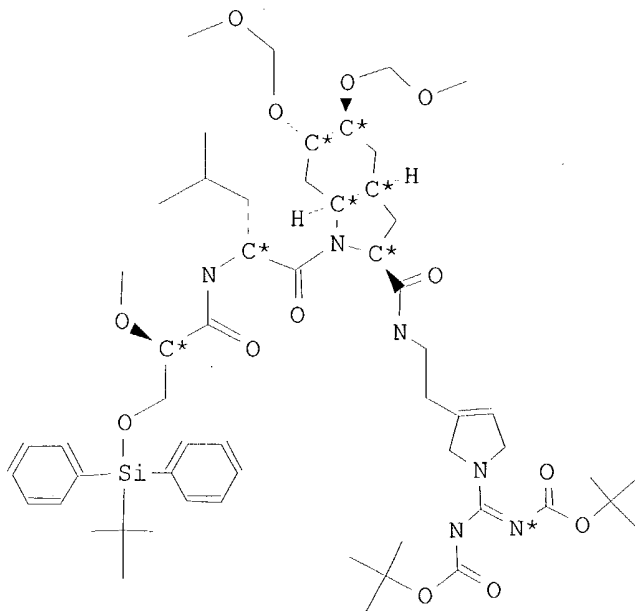
## Reaction Details:

RX

Reaction RID (.RID): 9232324.1  
 Reaction Classification (.CL): Preparation  
 Reagent (.RGT): TFA  
 Solvent (.SOL): CH2Cl2  
 Time (.TIM): 6 hour(s)  
 Reference(s):  
 1. Hanessian, Stephen; Margarita, Roberto; Hall, Adrian; Johnstone, Shawn; Tremblay, Martin; Parlanti, Luca, J.Amer.Chem.Soc., CODEN: JACSAT, 124(45), <2002>, 13342 - 13343; BABS-6373650

L8 ANSWER 2 OF 3 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN): 9315558  
 Molecular Formula (MF): C56 H86 N6 O13 Si  
 Molecular Weight (MW): 1079.41  
 Compound Type (CTYPE): heterocyclic



## Reaction:

RX

Reaction ID (.ID): 9222715  
 Reactant BRN (.RBRN): 9311441, 9282636  
 Reactant (.RCT): 1-<2-<3-(tert-butyl-diphenyl-silanyloxy)-2-methoxy-propionylamino>-4-methyl-pentanoyl>-5,6-bis-methoxymethoxy-octahydro-indole-2-carboxylic acid, <<3-(2-amino-ethyl)-2,5-dihydro-pyrrol-1-yl>-tert-butoxycarbonylimino-methyl>-carbamic acid tert-butyl ester  
 Product BRN (.PBRN): 9315558  
 Product (.PRO): C56H86N6O13Si  
 No. of React. Details (.NVAR): 1

## Reaction Details:

RX

Reaction RID (.RID): 9222715.1  
 Reaction Classification (.CL): Preparation  
 Reagent (.RGT): EDC, HOBT  
 Solvent (.SOL): CH2Cl2  
 Reference(s):

1. Hanessian, Stephen; Margarita, Roberto; Hall, Adrian; Johnstone, Shawn; Tremblay, Martin; Parlanti, Luca, J.Amer.Chem.Soc., CODEN: JACSAT,

124(45), &lt;2002&gt;, 13342 - 13343; BABS-6373650

## Reaction:

RX

Reaction ID (.ID): 9232193  
Reactant BRN (.RBRN): 9315558  
Reactant (.RCT): C56H86N6O13Si  
Product BRN (.PBRN): 9313827  
Product (.PRO): (tert-butoxycarbonylimino-<3-<2-(<1-<2-(3-hydroxy-2-methoxy-propionylamino)-4-methyl-pentanoyl>-5,6-bis-methoxymethoxy-octahydro-indole-2-carbonyl>-amino)-ethyl>-2,5-dihydro-pyrrol-1-yl>-methyl)-carbamic acid tert-butyl ester

No. of React. Details (.NVAR): 1

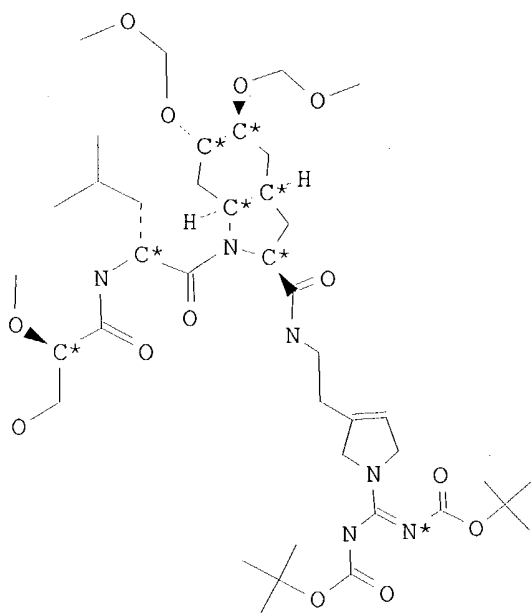
## Reaction Details:

RX

Reaction RID (.RID): 9232193.1  
Reaction Classification (.CL): Preparation  
Reagent (.RGT): TBAF  
Solvent (.SOL): tetrahydrofuran  
Reference(s):  
1. Hanessian, Stephen; Margarita, Roberto; Hall, Adrian; Johnstone, Shawn; Tremblay, Martin; Parlanti, Luca, J.Amer.Chem.Soc., CODEN: JACSAT, 124(45), <2002>, 13342 - 13343; BABS-6373650

L8 ANSWER 3 OF 3 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN): 9313827  
Chemical Name (CN): (tert-butoxycarbonylimino-<3-<2-(<1-<2-(3-hydroxy-2-methoxy-propionylamino)-4-methyl-pentanoyl>-5,6-bis-methoxymethoxy-octahydro-indole-2-carbonyl>-amino)-ethyl>-2,5-dihydro-pyrrol-1-yl>-methyl)-carbamic acid tert-butyl ester  
Autonom Name (AUN): (tert-butoxycarbonylimino-<3-<2-(<1-<2-(3-hydroxy-2-methoxy-propionylamino)-4-methyl-pentanoyl>-5,6-bis-methoxymethoxy-octahydro-indole-2-carbonyl>-amino)-ethyl>-2,5-dihydro-pyrrol-1-yl>-methyl)-carbamic acid tert-butyl ester  
Molecular Formula (MF): C40 H68 N6 O13  
Molecular Weight (MW): 841.01  
Compound Type (CTYPE): heterocyclic



## Reaction:

RX

Reaction ID (.ID): 9232193  
 Reactant BRN (.RBRN): 9315558  
 Reactant (.RCT): C56H86N6O13Si  
 Product BRN (.PBRN): 9313827  
 Product (.PRO): (tert-butoxycarbonylimino-<3-<2-(<1-<2-(3-hydroxy-2-methoxy-propionylamino)-4-methyl-pentanoyl>-5,6-bis-methoxymethoxy-octahydro-indole-2-carbonyl>-amino)-ethyl>-2,5-dihydro-pyrrol-1-yl>-methyl)-carbamic acid tert-butyl ester  
 No. of React. Details (.NVAR): 1

## Reaction Details:

RX

Reaction RID (.RID): 9232193.1  
 Reaction Classification (.CL): Preparation  
 Reagent (.RGT): TBAF  
 Solvent (.SOL): tetrahydrofuran  
 Reference(s):  
 1. Hanessian, Stephen; Margarita, Roberto; Hall, Adrian; Johnstone, Shawn; Tremblay, Martin; Parlanti, Luca, J.Amer.Chem.Soc., CODEN: JACSAT, 124(45), <2002>, 13342 - 13343; BABS-6373650

## Reaction:

RX

Reaction ID (.ID): 9194848  
 Reactant BRN (.RBRN): 9313827, 3704116  
 Reactant (.RCT): (tert-butoxycarbonylimino-<3-<2-(<1-<2-(3-hydroxy-2-methoxy-propionylamino)-4-methyl-pentanoyl>-5,6-bis-methoxymethoxy-octahydro-indole-2-carbonyl>-amino)-ethyl>-2,5-dihydro-pyrrol-1-yl>-methyl)-carbamic

Waller 10\_759667

acid tert-butyl ester, pyridine; compound  
with sulfur trioxide  
Product BRN (.PBRN): 9315975  
Product (.PRO): C40H68N6O16S\*C5H5N  
No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID): 9194848.1  
Reaction Classification (.CL): Preparation  
Reagent (.RGT): dibutyltin oxide  
Solvent (.SOL): CH2Cl2  
Time (.TIM): 6 hour(s)  
Reference(s):  
1. Hanessian, Stephen; Margarita, Roberto; Hall, Adrian; Johnstone, Shawn;  
Tremblay, Martin; Parlanti, Luca, J.Amer.Chem.Soc., CODEN: JACSAT,  
124(45), <2002>, 13342 - 13343; BABS-6373650

=>